Ensemble learning

Reminders/Comments

- Initial drafts due today
  - Some consternation about how open-ended it is
  - There are no specific requirements, so we will be more lenient. But you do have to justify your choices; if you can’t justify it, its likely a poor choice
  - Sample feedback
- Practice final released
- Review class next Thursday

How to give feedback

- It should look like an actual conference review:
- Summary of the paper/project
- Some positive feedback about what is done well
- Some constructive criticism about what needs to be improved
- Any other suggestions that can help out the person

Collections of models

- Have mostly discussed learning one single “best” model
  - best linear regression model
  - best neural network model
- Can we take advantage of multiple learned models?

Rationale

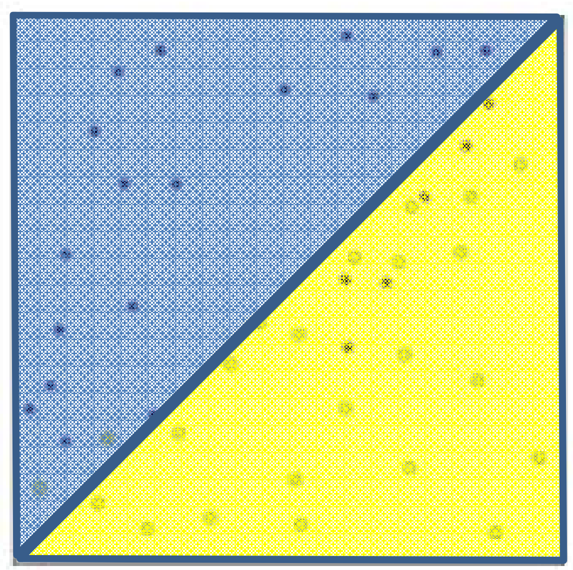
- There is no algorithm that is always the most accurate
- Different learners can use different
  - Algorithms (e.g., logistic regression or SVMs)
  - Parameters (e.g., regularization parameters)
  - Representations (e.g., polynomial basis or kernels)
  - Training sets (e.g., two different random subsamples of data)
- The problem: how to combine them

Ensembles

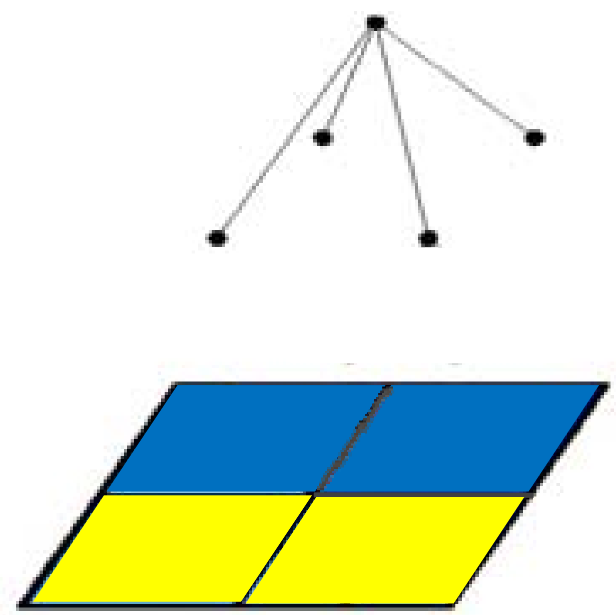
- Can a set of **weak learners** create a single strong learner?
- Answer: yes! See seminal paper: “The Strength of Weak Learnability” Schapire, 1990
- Why do we care?
  - can be easier to specify weak learners e.g., shallow decision trees, set of neural networks with smaller number of layers, etc.
  - fighting the bias-variance trade-off

Weak learners

- **Weak learners:** naive Bayes, logistic regression, decision stumps (or shallow decision trees)



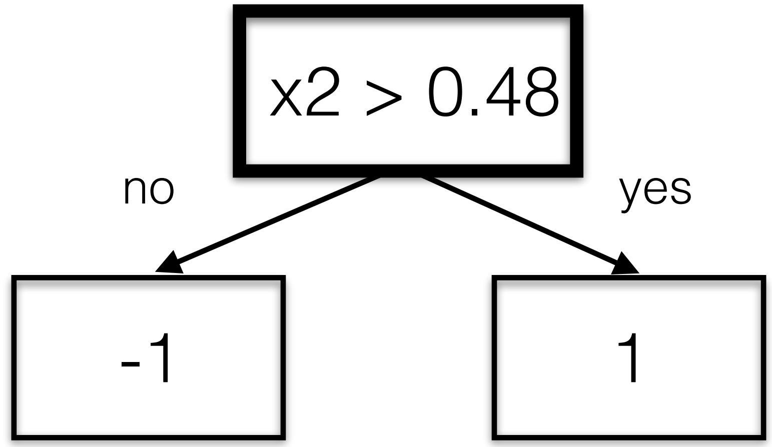
logistic regression



decision stump

*some material from slides by Eric Xing: http://www.cs.cmu.edu/~epxing/Class/10701-11f/Lecture/lecture22.pdf

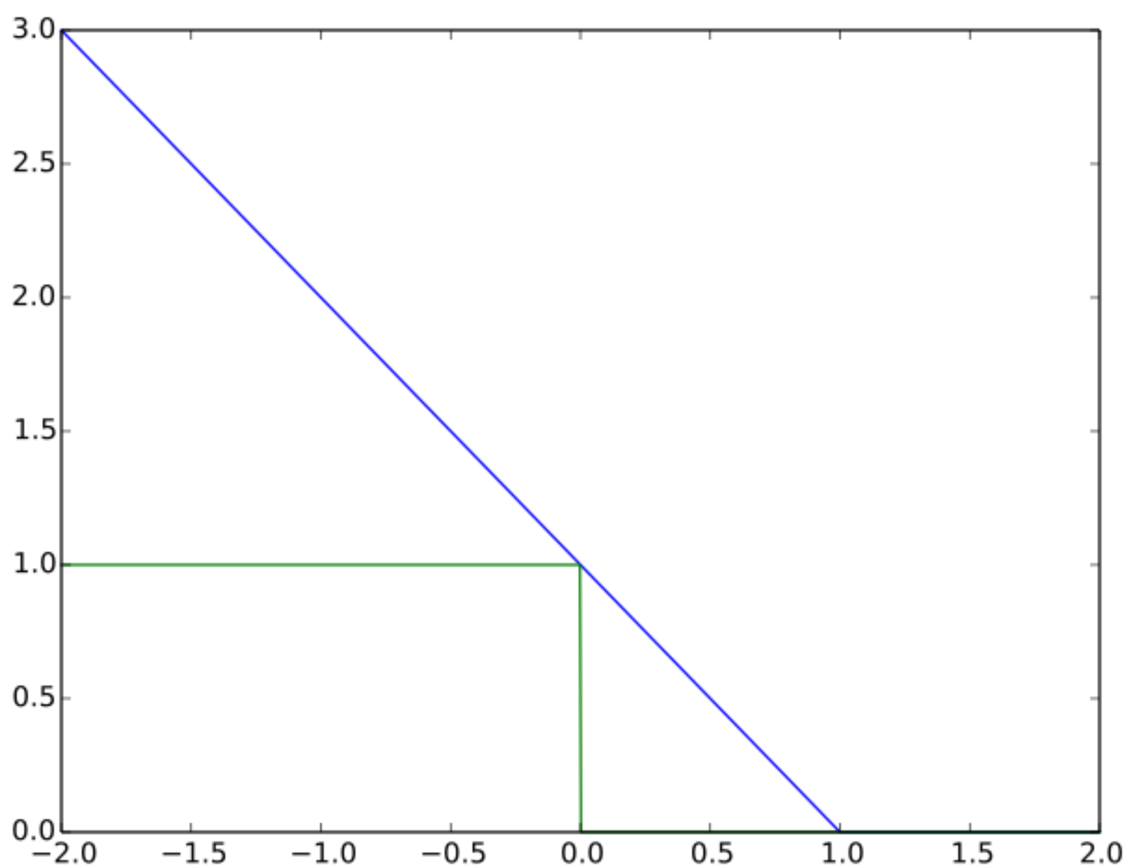
Example of a decision stump



Decision tree provides more splits;
decision stump is a one level decision tree

How learn signed prediction?

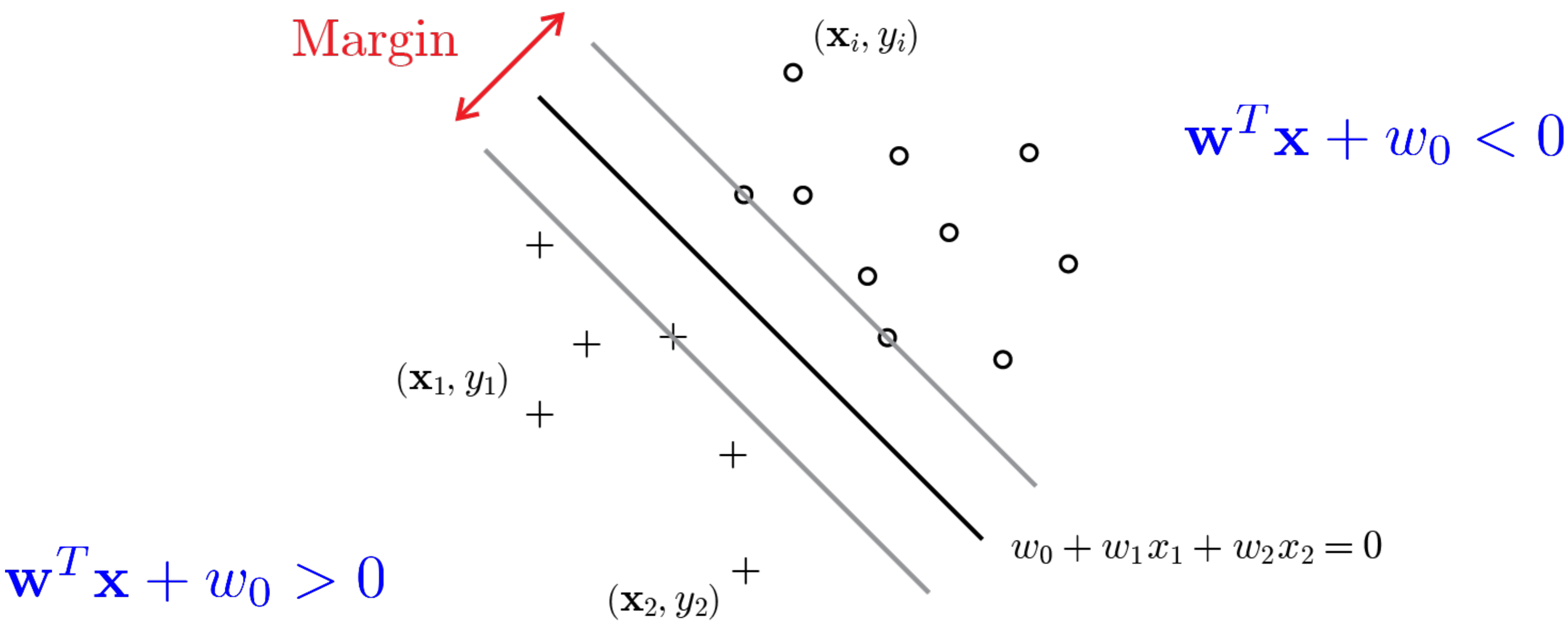
- Decision-stump outputs sign(<x, w>)
- Logistic regression and linear regression: take learned w, and prediction is set to sign(<x,w>)
- Support vector machines: minimize hinge loss



Green is zero-one loss
Blue is hinge loss

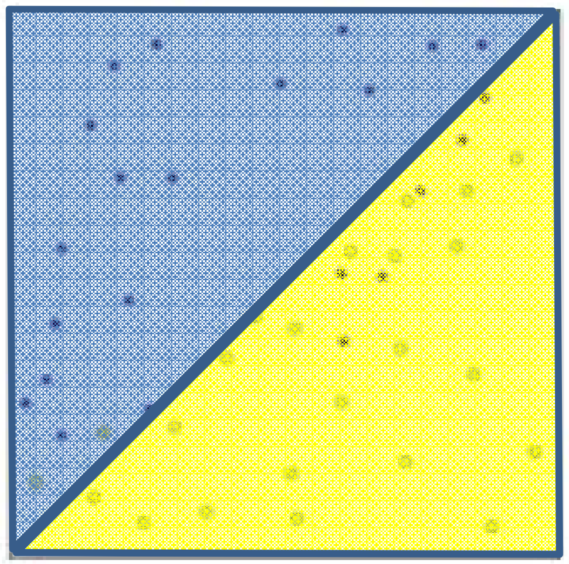
A side point about SVMs

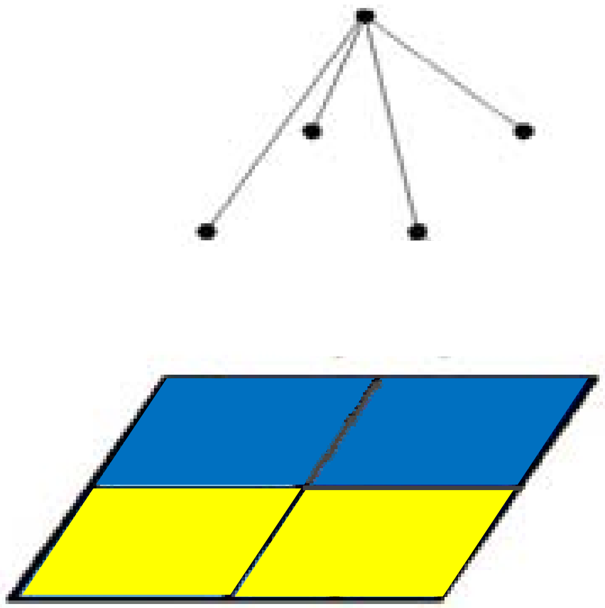
- Support vector machine: minimize hinge loss while also adding goal to maximize the margin



Weak learners

- **Weak learners:** naive Bayes, logistic regression, decision stumps (or shallow decision trees)





Are good ☺ - Low variance, don't usually overfit

Are bad ☹ - High bias, can't solve hard learning problems

*some material from slides by Eric Xing: http://www.cs.cmu.edu/~epxing/Class/10701-11f/Lecture/lecture22.pdf

Bias-variance tradeoff

- We encountered this trade-off for weights in linear regression
- Regularizing introduced bias, but reduced variance

$$\mathrm{MSE}(\hat{\theta}) = \mathrm{Var}(\hat{\theta}) + \left(\mathrm{Bias}(\hat{\theta}, \theta)\right)^2 .$$

- More generally, when picking functions

$$\mathrm{Var}(\hat{f}) + \mathrm{Bias}(\hat{f}, f)^2$$

How might you specify bias between functions?

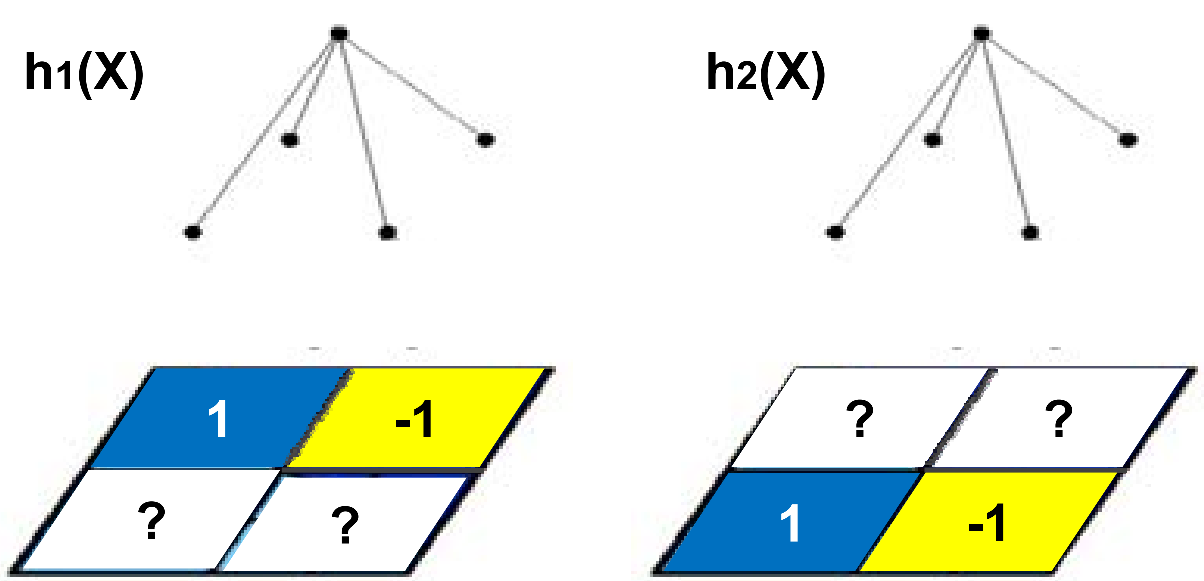
Voting (Ensemble methods)

- Instead of learning a single (weak) classifier, learn **many weak classifiers** that are **good at different parts of the input space**

- **Output class:** (Weighted) vote of each classifier

  Classifiers that are most "sure" will vote with more conviction

  Classifiers will be most "sure" about a particular part of the space. On average, do better than single classifier!



$H: X \rightarrow Y$ (-1,1)

$H(X) = h_1(X)+h_2(X)$

$H(X) = \text{sign}(\sum_t \alpha_t h_t(X))$

weights

Voting (Ensemble methods)

- Instead of learning a single (weak) classifier, learn **many weak classifiers** that are **good at different parts of the input space**

- **Output class:** (Weighted) vote of each classifier
  Classifiers that are most "sure" will vote with more conviction
  Classifiers will be most "sure" about a particular part of the space On average, do better than single classifier!

- **But how do you**
  force classifiers h_t to learn about different parts of the input space? weight the votes of different classifiers? α_t

Boosting [Schapire 89]

- **Idea:** given a weak learner, run it multiple times on (reweighted) training data, then let learned classifiers vote

- On each iteration *t*:
  - weight each training example by how incorrectly it was classified
  - Learn a weak hypothesis – h_t
  - Obtain a strength for this hypothesis – α_t

- Final classifier: $\boxed{H(X) = \text{sign}(\sum \alpha_t h_t(X))}$

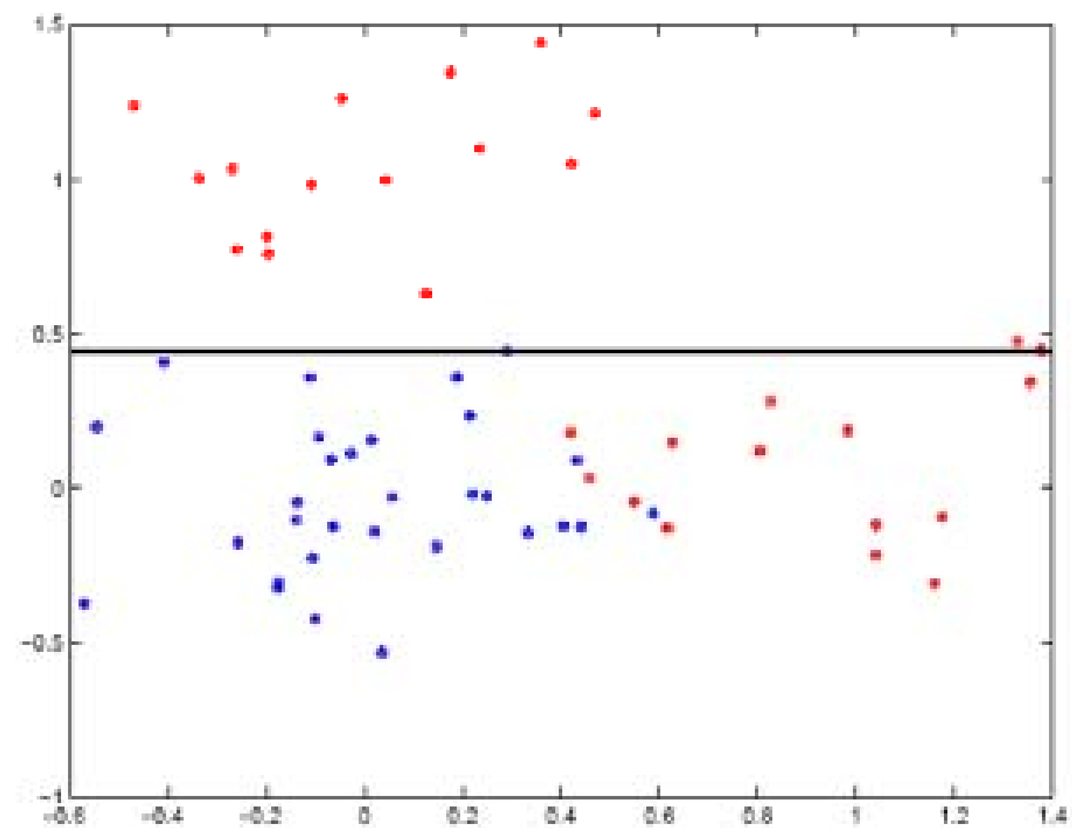
Combination of classifiers

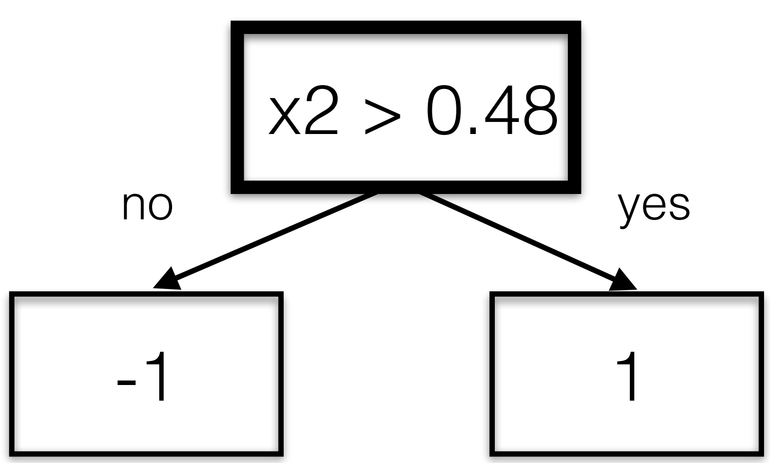
- Suppose we have a family of component classifiers (generating ±1 labels) such as decision stumps:

$$h(x;\theta) = \mathrm{sign}\left(wx_k + b\right)$$

where $\theta = \{k,w,b\}$

- Each decision stump pays attention to only a single component of the input vector





w = 1, k = 2, b = 0.48

Combination of classifiers

- We'd like to combine the simple classifiers additively so that the final classifier is the sign of

$$\hat{h}(\mathbf{x}) = \alpha_1 h(\mathbf{x};\theta_1) + \ldots + \alpha_m h(\mathbf{x};\theta_m)$$

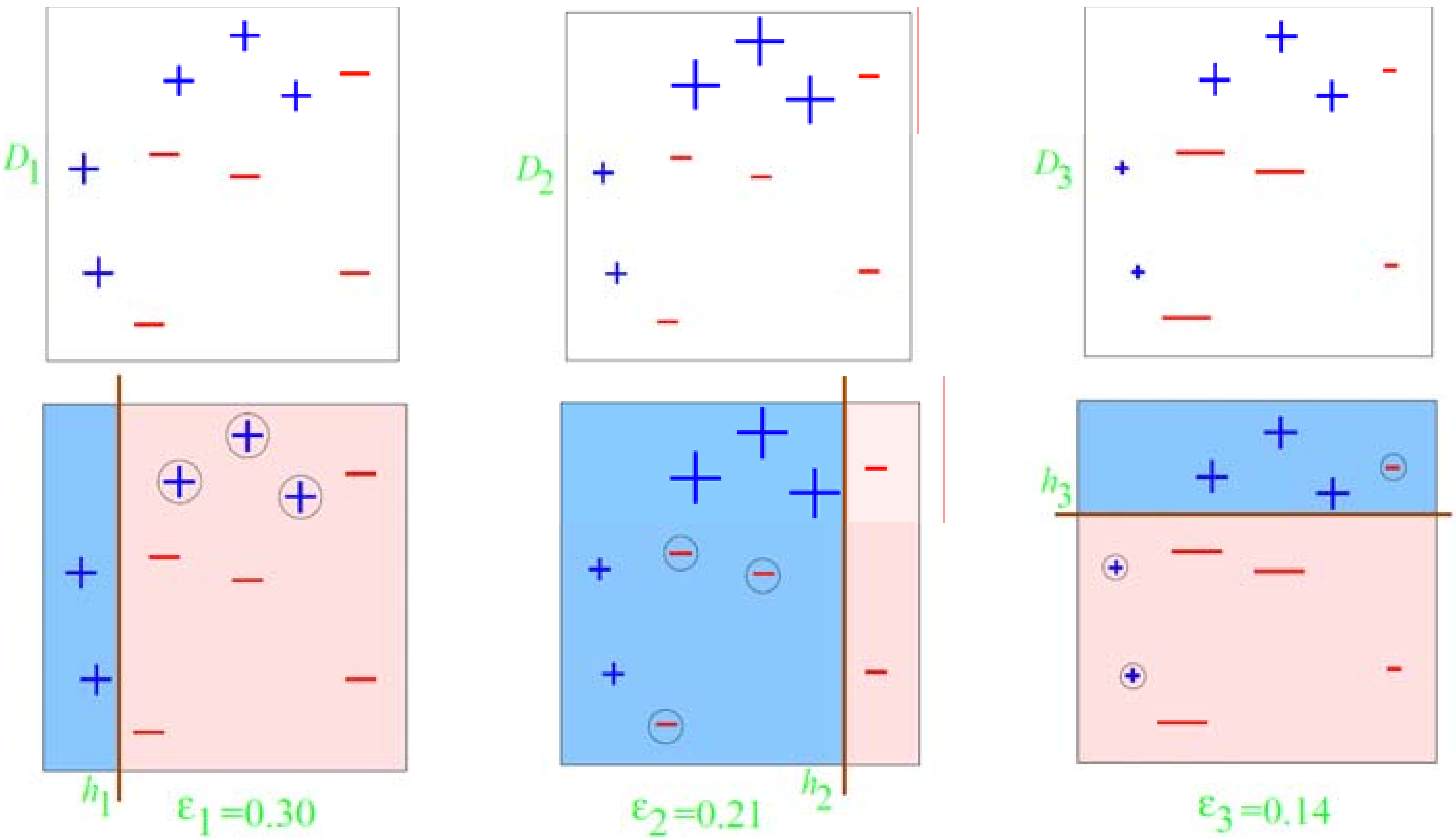
where the "votes" $\{\alpha_i\}$ emphasize component classifiers that make more reliable predictions than others

Recall

- On each iteration *t*:
  - weight each training example by how incorrectly it was classified
  - Learn a weak hypothesis – h_t
  - Obtain a strength for this hypothesis – α_t

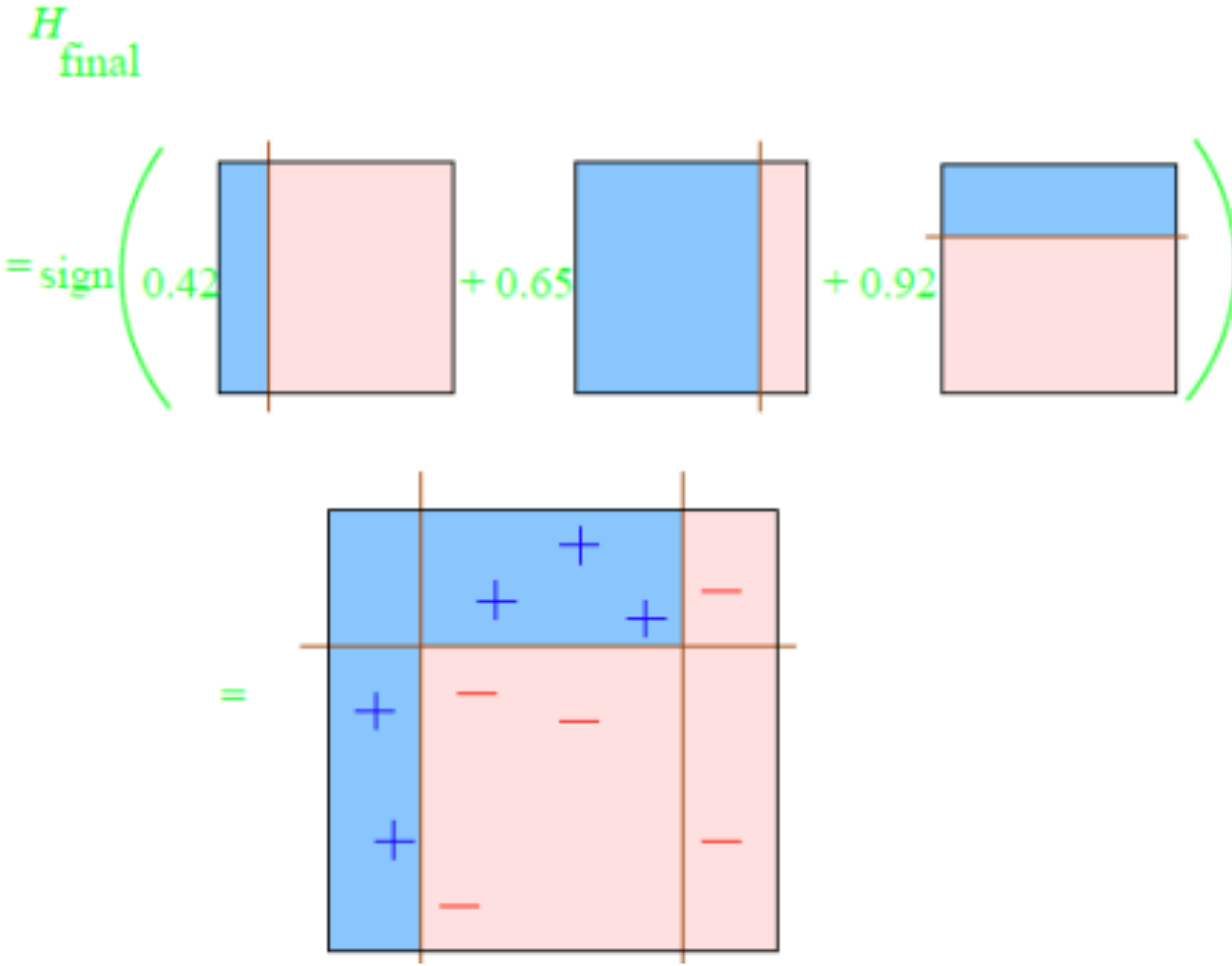
Boosting example with decision stumps

d = 2
n = 10



$\alpha_1 = 0.42$ $\alpha_2 = 0.65$ $\alpha_3 = 0.92$

Boosting example with decision stumps



AdaBoost

- **Input:**
  - N examples $S_N = \{(x_1,y_1),\ldots, (x_N,y_N)\}$
  - a weak base learner $h = h(x,\theta)$
- **Initialize:** equal example weights $w_i = 1/N$ for all $i = 1..N$
- **Iterate for $t = 1\ldots T$:**
  1. train base learner according to weighted example set (w_t, x) and obtain hypothesis $h_t = h(x,\theta_t)$
  2. compute hypothesis error ε_t
  3. compute hypothesis weight α_t
  4. update example weights for next iteration w_{t+1}
- **Output:** final hypothesis as a linear combination of h_t

Adaboost

- At the kth iteration we find (any) classifier $h(\mathbf{x};\, \theta_k^*)$ for which the weighted classification error:

$$\varepsilon_k = \sum_{i=1}^{n} W_i^{k-1} I(y_i \neq h(\mathbf{x}_i;\theta_k^*)) \Big/ \sum_{i=1}^{n} W_i^{k-1}$$

  is better than chance.
  - This is meant to be "easy" --- weak classifier
- Determine how many “votes” to assign to the new component classifier:

$$\alpha_k = 0.5 \log\left((1-\varepsilon_k)/\varepsilon_k\right)$$

  - stronger classifier gets more votes

epsilon small,
(1-epsilon)/epsilon is big
epsilon = 0.5 (random),
alpha = 0

- Update the weights on the training examples:

$$W_i^k = W_i^{k-1} \exp\{-y_i a_k h(\mathbf{x}_i;\theta_k)\}$$

$$W_i^k = \exp(-y_i f(x_i)) \qquad f(\cdot) = \sum_{j=1}^{k} \alpha_k h(\cdot\, ;\theta_k)$$

Base learners

- Weak learners used in practice:
  - Decision stumps
  - Decision trees (e.g. C4.5 by Quinlan 1996)
  - Multi-layer neural networks
  - Radial basis function networks
- Can base learners operate on weighted examples?
  - In many cases they can be modified to accept weights along with the examples
  - In general, we can sample the examples (with replacement) according to the distribution defined by the weights

Exercise

- How can we modify logistic regression with kernel features to use different weights for each example?

- Can we modify naive Bayes to use different weights for each example? How might we go about checking this?

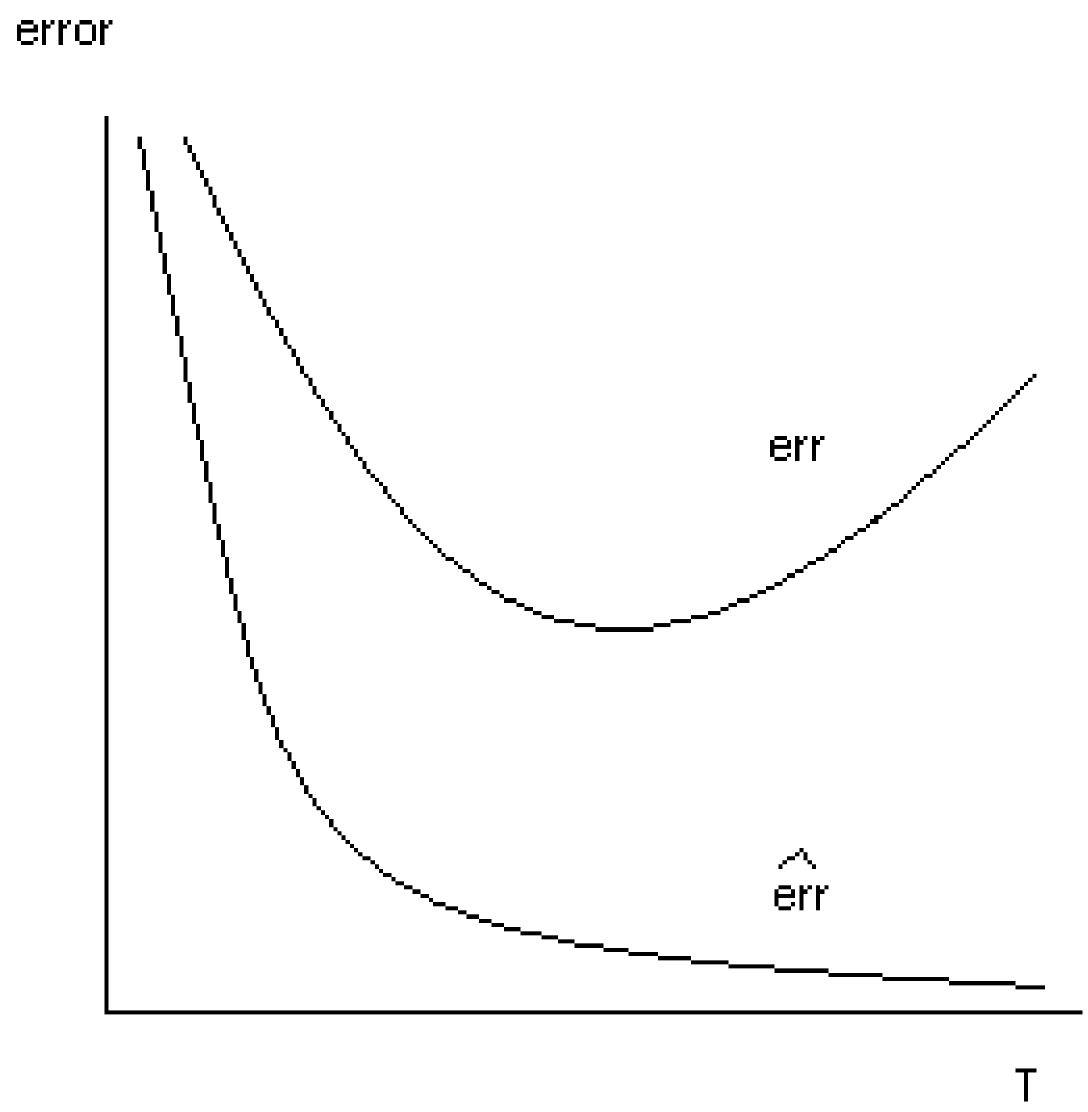
Generalization error bounds for Adaboost

$$error_{true}(H) \leq error_{train}(H) + \tilde{O}\left(\sqrt{\frac{Td}{m}}\right)$$

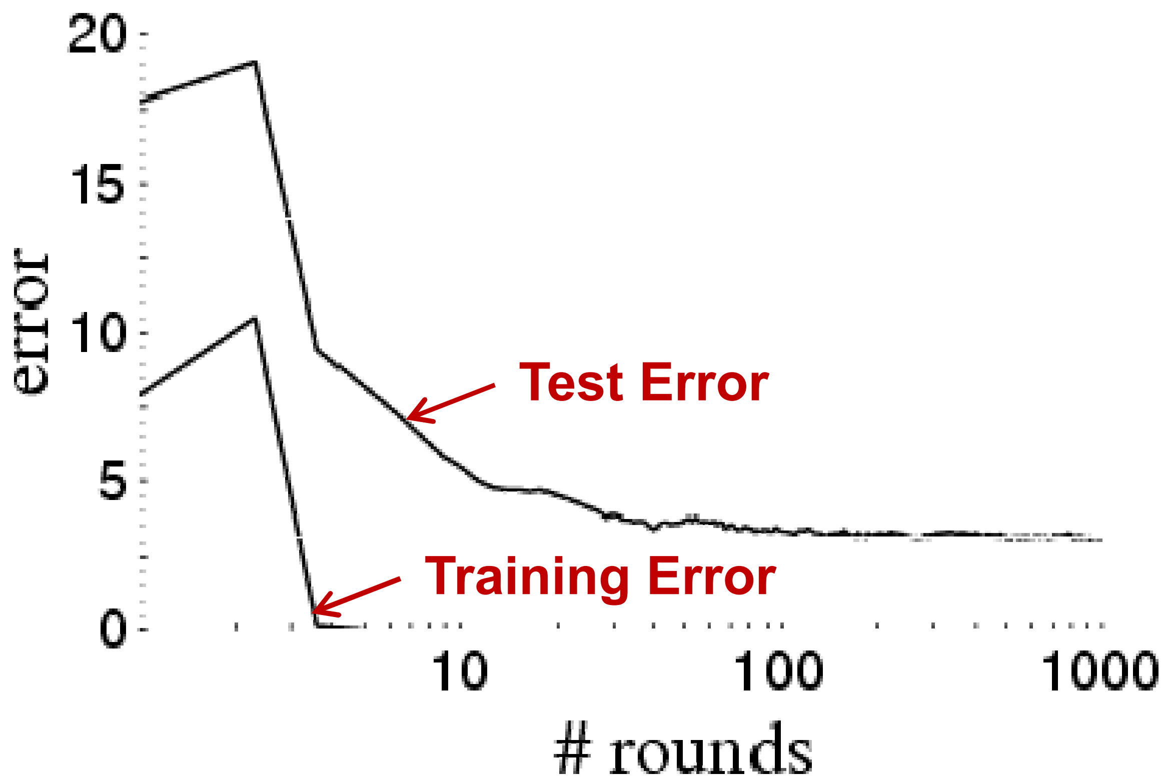
	bias	variance	
tradeoff	large	small	T small
	small	large	T large

- T – number of boosting rounds
- d – VC dimension of weak learner, measures complexity of classifier
- m – number of training examples

Expected Adaboost behavior due to overfitting



Adaboost in practice



- Boosting often, **but not always**
  - Robust to overfitting
  - Test set error decreases even after training error is zero

Why does this seem to contradict the generalization bound?

Intuition

- Even when training error becomes zero, the confidence in the hypotheses continues to increase

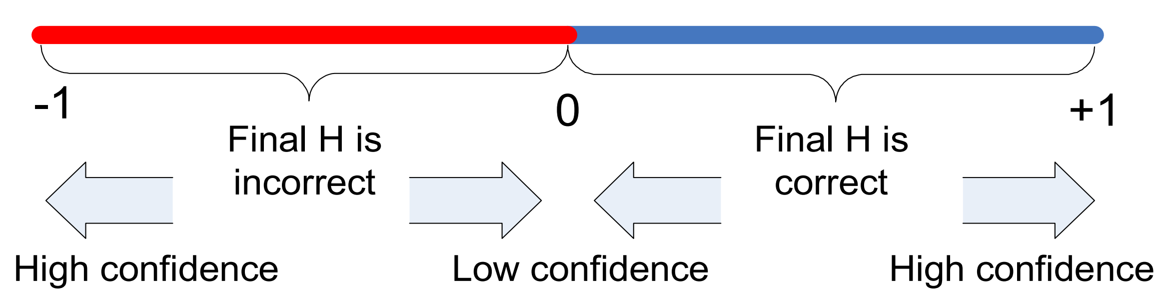
- Large margin in training (increase in confidence) reduces the generalization error (rather than causing overfitting)

- Quantify with margin bound, to measure confidence of a hypothesis: when a vote is taken, the more predictors agreeing, the more confident you are in your prediction

Margin

$$\begin{aligned} \text{margin}(x, y) &= y f(x) \\ &= y \sum_t a_t h_t(x) \\ &= \sum_t a_t y h_t(x) \\ &= \sum_{t:h_t(x)=y} a_t - \sum_{t:h_t(x)\neq y} a_t \end{aligned}$$

where y is the correct label of instance x, and a_t is a normalized version of α_t such that $\alpha_t \geq 0$ and $\sum_t a_t = 1$. The expression $\sum_{t:h_t(x)=y} a_t$ stands for the weighted fraction of correct votes, and $\sum_{t:h_t(x)\neq y} a_t$ stands for the weighted fraction of incorrect votes. Margin is a number between -1 and 1 as shown in Figure 4.



* from http://www.cs.princeton.edu/courses/archive/spr08/cos511/scribe_notes/0305.pdf

Margins and Adaboost

- AdaBoost increases the margins

- Bigger gamma is better for second term; gamma can be bigger if margin is bigger

$$\Pr_{\text{test}}(\text{margin}(\mathbf{x}, y) \leq 0) \; < \; \Pr\left(\text{margin}_h(\mathbf{x}, y) \leq \gamma\right) + O\left(\sqrt{\frac{d}{m\gamma^2}}\right)$$

Robert E. Schapire, Yoav Freund, Peter Bartlett and Wee Sun Lee. Boosting the margin: A new explanation for the effectiveness of voting methods. *The Annals of Statistics*, 26(5):1651-1686, 1998.

- It does not depend on T!!!

The number of boosting rounds

General Boosting

- "Boosting algorithms as gradient descent", Mason et al, 2000
- Adaboost is only one of many choices, with exponential loss
- Other examples and comparison: see "Cost-sensitive boosting algorithms: Do we really need them?" Nikolaou et al., 2016
- Main idea: given some loss L, (implicit) set of hypotheses and a weak learning algorithm,
  - generate hypothesis ht that point in a descent direction
  - assign weight relative to how much pointing in descent direction

Boosting and logistic regression

Logistic regression equivalent to minimizing log loss

$$\sum_{i=1}^{m} \ln(1 + \exp(-y_i f(x_i)))$$

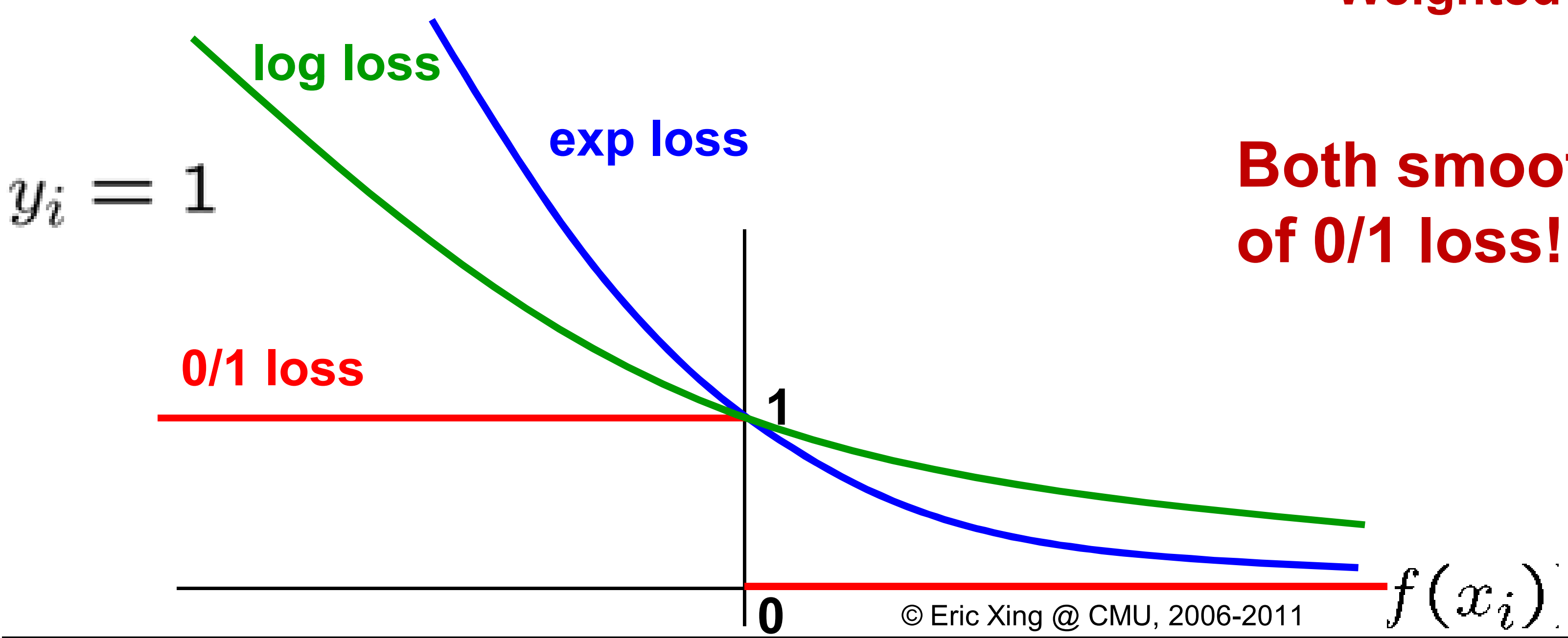
$$f(x) = w_0 + \sum_j w_j x_j$$

Boosting minimizes similar loss function!!

$$\frac{1}{m} \sum_{i=1}^{m} \exp(-y_i f(x_i))$$

$$f(x) = \sum_t \alpha_t h_t(x)$$

Weighted average of weak learners



Both smooth approximations of 0/1 loss!

Any Boost

Algorithm 1 : AnyBoost

Require :
- An inner product space $(\mathcal{X}, \langle , \rangle)$ containing functions mapping from X to some set Y.
- A class of base classifiers $\mathcal{F} \subseteq \mathcal{X}$.
- A differentiable cost functional $C\colon \operatorname{lin}(\mathcal{F}) \to \mathbb{R}$.
- A weak learner $\mathcal{L}(F)$ that accepts $F \in \operatorname{lin}(\mathcal{F})$ and returns $f \in \mathcal{F}$ with a large value of $-\langle \nabla C(F), f \rangle$.

Let $F_0(x) := 0$.
for $t := 0$ to T **do**
  Let $f_{t+1} := \mathcal{L}(F_t)$.
  if $-\langle \nabla C(F_t), f_{t+1} \rangle \leq 0$ **then**
    return F_t.
  end if
  Choose w_{t+1}.
  Let $F_{t+1} := F_t + w_{t+1} f_{t+1}$
end for
return F_{T+1}.

Can be thought of as a stepsize

How does AdaBoost fit into this?

(see “Boosting algorithms as gradient descent”, Mason et al, 2000)

AdaBoost as AnyBoost

- Loss function is the exponential loss

$$C(F) := \frac{1}{m} \sum_{i=1}^{m} c(y_i F(x_i))$$

$$-\langle \nabla C(F), f \rangle = -\frac{1}{m^2} \sum_{i=1}^{m} y_i f(x_i) c'(y_i F(x_i)).$$

- Such an f corresponds to minimizing a weighted error with weights

$$\frac{c'(y_i F(x_i))}{\sum_{i=1}^{m} c'(y_i F(x_i))}$$

Diversity of the ensemble

- An important property appears to be diversity of the ensemble
- We get to define the hypothesis space: does not have to be homogenous (e.g., the set of linear classifiers)
- Strategies to promote this include:
  - using different types of learners (e.g., naive Bayes, logistic regression and decision trees)
  - pruning learners that are similar
  - random learners, which are more likely to be different than strong/deliberate algorithms which might learn similar predictions

Exercise: Can boosting be used for regression?

Algorithm 1 : AnyBoost

Require :
- An inner product space $(\mathcal{X}, \langle , \rangle)$ containing functions mapping from X to some set Y.
- A class of base classifiers $\mathcal{F} \subseteq \mathcal{X}$.
- A differentiable cost functional $C\colon \operatorname{lin}(\mathcal{F}) \to \mathbb{R}$.
- A weak learner $\mathcal{L}(F)$ that accepts $F \in \operatorname{lin}(\mathcal{F})$ and returns $f \in \mathcal{F}$ with a large value of $-\langle \nabla C(F), f \rangle$.

Let $F_0(x) := 0$.
for $t := 0$ to T **do**
  Let $f_{t+1} := \mathcal{L}(F_t)$.
  if $-\langle \nabla C(F_t), f_{t+1} \rangle \leq 0$ **then**
    return F_t.
  end if
  Choose w_{t+1}.
  Let $F_{t+1} := F_t + w_{t+1} f_{t+1}$
end for
return F_{T+1}.

If so, whats the loss?
How might this pseudocode change?